Chemistry and structure in Acta Crystallographica Section C

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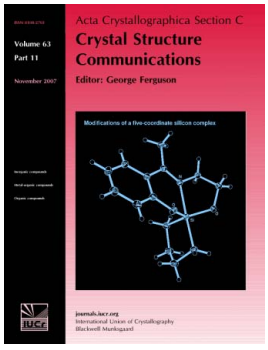

Acta Crystallographica Section C: Structural Chemistry specializes in the rapid dissemination of high-quality detailed studies of novel and challenging crystal and molecular structures of interest in the fields of chemistry, biochemistry, mineralogy, pharmacology, physics and materials science. The unique checking, editing and publishing facilities of the journal ensure the highest standards of structural reliability and presentation, while providing for reports on studies involving special techniques or difficult crystalline materials. Papers go beyond reporting the principal numerical and geometrical data, and may include the discussion of multiple related structures, a detailed description of non-routine structure determinations, placing the structure in an interesting scientific, physical or chemical context, or the discussion of interesting physical properties or modes of association. Reports of difficult or challenging structures, such as cases of twinning, severe disorder, or diffuse solvent regions are welcomed, provided the presented structures are correct and the difficulties and strategies used to treat them are scientifically discussed and properly documented. *Section C* readers have access to an extensive back archive of high-quality structural data.

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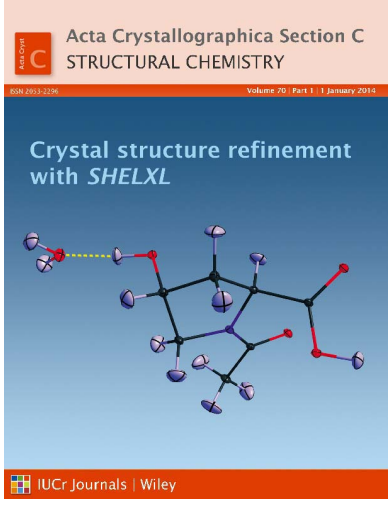
Acta Crystallographica Section C is continuing its transition to a journal that publishes exciting science with structural content, in particular important results relating to the chemical sciences. *Section C* is the journal of choice for the rapid publication of articles that highlight interesting research facilitated by the determination, calculation or analysis of structures of any type, other than macromolecular structures. Articles that emphasize the science and the outcomes that were enabled by the study are particularly welcomed. Authors are encouraged to include mainstream science in their papers, thereby producing manuscripts that are substantial scientific well-rounded contributions that appeal to a broad community of readers and increase the profile of the authors.

One change that readers of the journal will notice in the near future is that the journal's website (**journals.iucr.org/c**) will be redesigned completely. This will enable highlighting of the most recent significant articles on the homepage and easy navigation to articles for readers, while making all necessary information for prospective authors readily accessible.

As part of the transition, the journal aims to publish special issues on a regular basis. In February 2014, a special issue on *Computational Materials Discovery* was published and attracted considerable attention and downloads. A virtual issue on *Coordination Polymers* was also published in July 2014. Two more special issues are in the pipeline: one on *The Structural Chemistry of Homogeneous and Heterogeneous Catalysts* and one on *NMR Crystallography*. The latter is a rapidly emerging field and its importance to structural scientists was recently recognized by the establishment of the **IUCr Commission on NMR Crystallography and Related Methods** during the 2014 IUCr Congress in Montreal. It is hoped that *Section C* can become a leading journal for the publication of results relating to this field.

In conjunction with the new outlook of the journal, it was decided to add a second Main Editor to the editorial board. I am delighted to welcome Paul Raithby from the University of Bath, UK, as a Main Editor. Paul's reputation and network in the chemistry and crystallography communities make him an invaluable addition to the team and will bolster the journal's interface with the chemistry community.

To further promote awareness of the expansion of the scope of *Section C* to cover all areas of Structural Chemistry, in August 2014 representatives of the journal were present at the ACS Fall Meeting in San Francisco to promote this fact. It is anticipated that *Section C* will have a presence in 2015 at further Chemistry-focused meetings, such as the 12th International Conference on Materials Chemistry, University of York, UK (20–23 July, 2015) and IUPAC-2015, Busan, Korea (9–14 August, 2015).



We are excited to present two must-read articles in this issue, which are of particular interest for the structural chemistry community. The first describes the new features in the 2014 version of the highly popular structure refinement program *SHELXL* [G. M. Sheldrick (2015). *Acta Cryst.* C**71**, 3–8]. The new features include improved restraint options, easier disorder handling, advances in absolute structure determination and inclusion of more comprehensive information in the generated CIF, to mention just a few. The advances in the program make it highly worthwhile for users to upgrade to the newest version and this journal strongly recommends its use for future work. The second article describes in detail the current implementation of the SQUEEZE procedure in the program *PLATON* for dealing with hard-to-model disordered species, usually solvent, in a structure [A. L. Spek (2015). *Acta Cryst.* C**71**, 9–18]. This technique has been available for many years, but has recently been modified to allow the contribution to the structure factors of the omitted disordered component to be included in F_{calc}, rather than being subtracted from I_{obs}, thereby retaining the integrity of the original intensity data file. This

has been made possible by modifications incorporated into the new version of *SHELXL*. Both papers are highly recommended reading.

Authors are reminded that it is possible to submit the body of a manuscript as a **Word** document, if preferred, rather than writing the entire paper in the CIF itself. Then only the structural data parts of the work still need to be submitted as a CIF. Alternatively, the easy-to-use *publCIF* software available from the journal website can be used to assist creation of the final CIF, with or without the text sections, for submission.

Several *Section C* Co-editors retired at the IUCr Congress last August and it is my pleasure to record here my sincere appreciation of their dedication and efforts beyond the call of duty, their professionalism and their support of the journal. The retirees are: Ricardo Baggio, Mark Elsegood, George Ferguson, Ilia Guzei, Marcia Scudder and Amber Thompson.

I welcome Filipe Paz (University of Aveiro, Portugal), Chris Frampton (Brunel University, UK), Tong-Bu Lu (Sun Yat-Sen University, China), Noël Lugan (Laboratoire de Chimie de Coordination du CNRS, Toulouse, France) and Yoshiki Ohgo (Teikyo University, Japan) to the Co-editorial team and look forward to working closely with them over the coming years. All current *Section C* Co-editors and the Chester Editorial Office staff are warmly thanked for their ongoing dedicated support and contributions to the daily operations of the journal.